One-dimensional turbulence modeling of soot formation and transport in non-premixed turbulent flames

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Abstract: *Soot modeling in turbulent flames involves tightly coupled problems of combustion chemistry, particle transport, compressible fluid dynamics, and turbulence behavior in addition to soot chemistry and transport. Significant uncertainties accompany soot modeling and transport in such systems, hindering progress toward accurate combustion models and predictive simulation tools. The one-dimensional turbulence (ODT) model, using a stochastic approach to turbulence modeling, captures the full range of length and time scales in a simulation and provides detailed statistical data of the flow configuration, chemistry, and particle transport. Previously, ODT has demonstrated accuracy and computational efficiency compared to direct numerical simulation (DNS) of turbulent, non-premixed flames. We present ODT simulations of soot behavior and transport in non-premixed ethylene jet flames, representing late-flame regions and parameter spaces typically inaccessible to DNS. The simulation configurations are based on experimental cases presented by the International Sooting Flame (ISF) Workshop, readily accessible online. We focus on soot chemistry and particle transport by implementing advanced soot models and quantifying gas temperature and soot volume fraction in order to evaluate the models used and gain insight into the nature of soot-flame interactions. Our simulations stimulate progress toward parametric studies of soot behavior and more comprehensive modeling.*

Keywords: ***soot, one-dimensional turbulence, turbulent non-premixed flames***

1. Introduction

Most practical combustion processes involve turbulent, non-premixed flames, which produce soot. Soot is responsible for a flame's luminosity, generates a large portion of a flame's radiative heat transfer to its surroundings, and contributes to many of the health and safety hazards associated with air pollution from combustion systems [1, 2]. Accurate soot modeling is crucial to developing predictive simulation tools, but current models suffer from significant uncertainties. Soot formation and growth depends heavily on the surrounding gas temperature and composition, which in turn depend on radiative heat transfer occurring within a flame, much of which is generated and affected by the presence of soot particles. While gaseous species can reach a near-equilibrium state almost instantaneously under typical combustion conditions, soot particles are extremely large in comparison and move slowly; as a result, they cannot be modeled using the same assumptions. Additionally, their presence further widens the range of length and time scales involved and introduces new interactions [3]. To simulate sooting flames accurately, researchers must account for both the physical models of soot chemistry and the increased range of scales involved, both of which can increase complexity significantly.

Soot chemistry comprises two main categories of physical behavior: first, molecular-scale reactions that contribute to primary particle formation; and second, coagulation of polycyclic aromatic hydrocarbons (PAH) and small particles to form large soot aggregates. Early soot modeling combined the two categories, using semi-empirical kinetic expressions to approximate soot formation and growth [4, 5]. In general, such models represent soot behavior under certain conditions using relatively simple expressions, and they are commonly used in simulations where simple chemistry is adequate [6, 7]. More detailed soot mechanisms

often treat the two categories of behavior separately, linking them at the transition between the molecular chemistry of individual PAH molecules and the aggregation of the smallest soot particles, somewhat arbitrarily defined. While the contribution of individual gaseous species and elementary reactions to soot particle nucleation and growth is unclear, acetylene-based nucleation mechanisms are strongly supported by experimental evidence [8–10] and perform well compared to more complicated mechanisms [5, 11–16]. PAH-based nucleation and surface growth mechanisms offer higher accuracy if the simulation uses a gas-phase chemical mechanism that includes PAH [17, 18], but such gas-phase mechanisms come at increased computational cost. Oxidation of soot particles is usually modeled in terms of attack by molecular oxygen and its radicals [19–22], but we may also encounter more complex phenomena like inner particle burning and oxidation-induced particle fragmentation [23–26].

Above an arbitrary particle size, using chemical reactions to describe soot behavior becomes prohibitively complex in all but the simplest systems. Instead, we use the soot particle size distribution (PSD) to describe the existing population of soot particles statistically. Monte Carlo and sectional methods approximate direct solutions but come at high computational cost [27–30]. The method of moments is advantageous and commonly used because it involves significantly fewer transport equations, but moment methods require closure, which can be achieved via quadrature [31], interpolation [32, 33], or any number of extended or hybrid moment methods [34–38]. Both soot chemistry models and PSD methods share a significant limitation: the more complex the model, the less computationally efficient it is and the more resources are required for the simulation. Even without modeling soot, combustion simulations can be incredibly complex and numerically taxing, so various simulation approaches must be explored.

Direct numerical simulations (DNS) resolve the full range of relevant length and time scales in a flow by directly solving the numerical Navier-Stokes equations. It has been applied to the early evolution of soot in flames [39–42], but because of its high computational cost, DNS is restricted to short simulation times, preventing study of soot evolution through the entire history of a flame. While it has helped identify some of the unsteady long time scales as well as the significance of mixture fraction diffusion in soot transport, its limitations restrict its use in studying late-flame phenomena, including the interactions between turbulence and soot oxidation, soot radiation and flame weakening, and soot emissions.

Large-eddy simulations (LES) combine direct resolution of grid-scale quantities with subgrid modeling to address some of the weaknesses present in DNS studies, but has its own problems. LES is more computationally affordable than DNS, but because it does not directly resolve fine dissipation-scale quantities, it requires subgrid models for combustion chemistry, turbulent flow, radiation heat transfer, and soot chemistry. Additionally, unresolved quantities are often parameterized in state space with empirical relationships or assumed distributions that lack universal applicability. In particular, soot behavior is tightly coupled to temperature and gas composition and involves an exceptionally wide range of length and time scales, which means that it cannot be captured using mixture fraction state relations as is often done with gaseous species. Nuances like this complicate soot modeling in LES, and it is common for LES studies of sooting flames to neglect subgrid soot fluctuations [43, 44] or differential diffusion between gas and soot [45, 46], which can lead to serious errors in predicting radiative heat transfer and temperature fields [47].

The one-dimensional turbulence (ODT) model uses a stochastic approach, directly resolving fine dissipation scales and using a stochastic turbulence model based on resolved

velocity fields at larger scales [48–51]. By doing so in only one dimension, ODT allows us to follow differential diffusion and detailed chemistry over the full flame evolution time with higher computational efficiency than DNS and greater accuracy than some LES. Like LES, ODT requires models for combustion chemistry and soot behavior, but it applies them at relatively large scales for which they were developed rather than the subgrid scales of LES, where model validation can be complex and difficult to achieve. ODT has successfully been used to study processes that require full resolution of the diffusive and chemical time scales such as extinction and reignition [52, 53] jet flames [54, 55], and buoyant fire plumes [56]. Most recently, ODT was expanded to include cylindrical and spherical formulations and applied to a round jet flame [57]. While ODT does not replace other turbulent simulation approaches like DNS and LES, its computational efficiency and resolution of a full range of length and time scales makes it a valuable complement to traditional simulation tools.

ODT has been successfully applied in several sooting jet flame configurations similar to the configuration in the present study [6, 56, 58, 59], including comparison to DNS of soot formation and transport in a nonpremixed ethylene jet flame [7]. Here, we present initial ODT simulations of a round, sooting ethylene jet flame in the experimental configuration of Zhang et al. [60]. We quantify gas temperature and soot volume fraction and compare it to experimental data alongside simulations of this configuration performed by other research groups. We will show that ODT, with the addition of advanced soot models, may be a valuable complement to LES in investigating fundamental soot behavior and transport, particularly in the area of parametric studies of soot mechanisms.

2. Model Description

This study employs the most current version of the ODT code as in Lignell et. al. [57], and the ODT model in general is described in detail in the literature [41, 48–50, 57]. The ODT code uses a Lagrangian finite-volume formulation for diffusive advancement, including adaptive mesh refinement [41]. In this approach, combustion dilation causes grid cells to increase or decrease in volume while mass remains constant within each cell. Turbulent advection is modeled with stochastic processes called "eddy events" that map functions on the domain via triplet maps. These eddy events occur concurrently with the solution of unsteady one-dimensional transport equations for mass, momentum, and enthalpy. In sooting flame cases, we also transport species mass fractions and soot particle size distribution properties. Because the ODT model is one-dimensional, it is limited to homogeneous or boundary-layer flows, such as jets, wakes, and mixing layers; these types of flows, however, are common in nature and central to turbulence research.

Turbulent advection punctuates diffusive advancement via eddy events whose sizes are drawn randomly from a sample distribution. A given eddy of size l and location x_0 has an eddy timescale t and an associated eddy rate $\frac{1}{t}$. Eddies occur as a Poisson process in accordance with their given rates and locations. Eddy events modify domain variables using triplet maps, as illustrated for a cylindrical domain in Figure 1. For a region of eddy size l, the domain is copied to create three map images, the three images are placed back to back with the middle image inverted to maintain continuity, and the composite is reapplied to the domain. This process applies to all transported variables on the domain. Applied properly, the triplet map increases scalar gradients and decreases length scales consistent with the application of turbulent eddies in real flows, while also conserving all quantities and their statistical moments and maintaining conti-

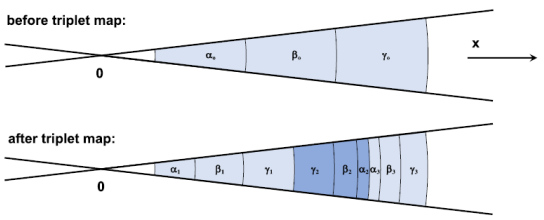

Figure 1: Schematic diagram of a cylindrical triplet map, adapted from [57]. Before the triplet map, the domain contains three grid cells of equal volume, while after the triplet map has been applied, the domain contains nine cells. The nine final cells are labeled according to the cells from which they originated and shaded to indicate that three map images were combined to create the final composite.

nuity in property profiles. Subsequent eddies in the same region will result in a cascade of scales, and eddy rates depend on eddy size and the local kinetic energy such that they follow turbulent cascade scaling laws.

Three ODT parameters further specify the eddy event process: the eddy rate parameter C scales the rate of occurrence of the eddy events; the viscous penalty parameter Z suppresses small eddy events; and the large eddy suppression parameter β constrains eddy events such that they do not reach over the elapsed simulation time. These parameters are user-specified and can be modified to adapt to various flow conditions. Further, ODT can be applied in planar, cylindrical, or spherical configurations and evolved in either a time or spatial coordinate according to the desired flow geometry and properties. For more detail on the configuration and equations used in the present study, please refer to Lignell et al. [57].

3. Simulation Configuration

The ODT simulations presented here are round, nonpremixed, turbulent ethylene jet flames based on the configurations given by Zhang et al. [60] using data reported by the International Sooting Flame (ISF) Workshop as "ISF-4 target flame 2: Sandia flame" [61]. ODT's cylindrical, spatially-evolving jet configuration has been validated by Lignell et al. [57] against experimental data for the methane jet flame described by Meier et al. [62], and its cylindrical, temporally-evolving configuration was tested by Starick et al. [63] against the experimental lifted methane jet given by Cabra et al. [64]. Both studies indicate that the cylindrical ODT formulation better predicts experimental behavior than the planar ODT formulation does in these cases. Neither of ODT's cylindrical formulations have yet been applied to the ISF-4 Sandia target flame presented here.

In the experimental configuration, a fuel stream of pure ethylene issues into an air coflow and piloted with an annular premixed ethylene-air flame. The fuel stream exits the jet at 294 K and 1 atm with a velocity of 54.7 m/s and a Reynolds number of 20,000. This assumes that the fuel has a kinematic viscosity of 8.6E-6 m^2/s. The coflow air stream also exits at 294 K and 1 atm, but with a velocity of 0.6 m/s. The pilot stream consists of ethylene and air at an equivalence ratio of 0.9 and a flow rate corresponding to 2% of the heat release of the main jet. The jet diameter is 3.2 mm and the pilot diameter is 19.1 mm. In the simulation, the jet dimensions and stream velocities were set at these values. For the cylindrical, temporally evolving configuration used here, the ODT parameters were set to $Z = 400$, $C = 5$, and $\beta = 5$ according to tuning based on non-sooting jet flames.

The gas chemistry is described by a reduced ethylene reaction mechanism containing 19 species and 167 reactions as described by Lignell et. al. [39, 65]. Gas radiation uses an optically thin model with Planck mean absorption coefficients. Soot chemistry is described by the four-step empirical model by Leung and Lindstedt [4], and the soot particle size distribution is closed by the quadrature method of moments [31] with four transported soot moments.

4. Results and Discussion

The Sandia jet configuration studied here is also being simulated by other research groups with various tools; they are summarized in Table 1 alongside the authors of this study. The purpose of comparing our data to theirs is simply to evaluate progress. No one research group or simulation approach captures all of the important features of the measured soot data for the Sandia case. Our goal is to show that ODT may be a suitable model for studying soot transport and behavior in jet flames alongside more traditional tools like LES.

Figure 2 compares results of the current study with published results from the other three groups listed in Table 1, including centerline gas temperature (top row) and centerline soot volume fraction (bottom row). As noted above, no one group or simulation approach captures all features of the experimental data. All groups obtained somewhat similar data predictions for temperature (top row of Figure , but no one group or simulation approach appears to capture all of the features of the soot volume fraction data. All of the simulations pictured here overpredict soot volume fraction, and each differs in its prediction of the location of the peak soot volume fraction.

The current study overpredicts soot volume fraction more than the other published studies, but predicts values within two orders of magnitude of the experimental data; additionally, the soot volume fraction curve lacks a defined peak. This can be attributed to the soot model used, the empirical, four-step kinetic model of Leung and Lindstedt [4]. Tests of this simulation case revealed that the mechanism does not predict the correct balance of soot formation and destruction, heavily favoring nucleation and growth over oxidation under the conditions of the experimental Sandia flame. That imbalance likely explains the high predicted soot volume fraction and the lack of a peak in the data. The Leung and Lindstedt model employed here is often used for simple predictions of soot chemistry, but its empirical approach and use of kinetic reaction steps limits its ability to capture or predict fundamental soot behavior. As such, it is an adequate starting point and a useful benchmark, but we cannot expect accurate comparisons to experimental soot volume fraction data.

The limitations of the Leung and Lindstedt model for this case prompted us to include other models for soot chemistry in the ODT code. In particular, the hydrogen-abstraction acetylene-addition (HACA) model offers a more physical description of soot particle growth and oxidation, but still has a relatively simple, acetylene-based reaction mechanism [13, 15, 16]. Additionally, there are several alternative models for oxidation by O_2 and OH [19–21] that modify or replace the Leung and Lindstedt expressions. There are also several alternative models for particle coagulation that better bridge the size gap between molecular chemistry and particle-particle interactions, including, notably, the Fuchs form of the Brownian coagulation coefficient [67, 68]. These mechanisms in particular were implemented in the ODT code and run in various combinations to ascertain the effects that each piece of the overall soot chemistry has on simulation results.

Table 2 summarizes four ODT simulation cases performed to this end. Aside from the soot mechanisms, each case uses identical ODT parameters, and all four cases share the same soot particle size distribution treatment, as detailed in Section 3. Figure 3 shows the results of those simulations alongside the experimental data for the Sandia target flame case. The centerline temperature profile is mostly unaffected by the changing soot mechanisms, but the centerline soot volume fraction f_v varies by several orders of magnitude above and below the experimental values. The oxidation mechanism appears to have particular importance. As discussed above, the Leung and Lindstedt mechanism underpredicts soot destruction via oxidation, and as such, we observe in Case A no de-

Table 1: Summary of groups simulating the Sandia ISF-4 Target Flame [61, 66], including the present study (rightmost column).

	Princeton (M. Mueller)	Imperial (ICL) (P.R. Lindstedt)	Cal Tech (G. Blanquart)	BYU (D.O. Lignell)
CFD	LES	RANS	LES	ODT
Turbulence	Dyn. Smagorinsky	SSG	Dyn. Smagorinsky	ODT
Combustion	Flamelet	Exp. chemistry	FPV	Direct
Soot PSD	HMOM	Sectional	Bivariate DQMOM	QMOM
Soot inception	PAH	Acetylene	PAH	Acetylene

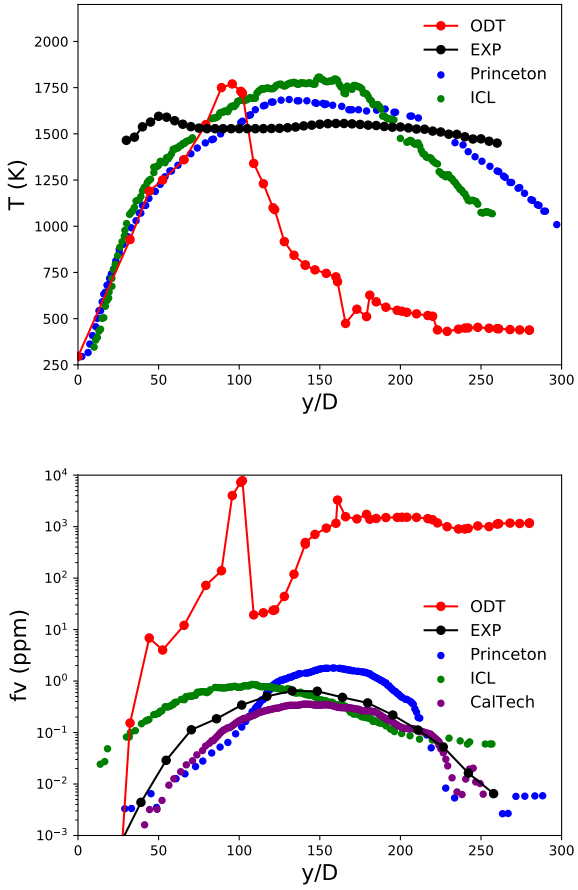

Figure 2: Results of the present ODT simulations of the Sandia ISF-4 Target Flame 2 [60] alongside data from three other research groups also simulating this flame, adapted from [61, 66].

crease in soot volume fraction high in the flame (above $y/D = 150$). The other two oxidation mechanisms, HACA and NSC/Neoh, both predict higher oxidation rates than the Leung and Lindstedt model does, so the soot volume fraction profiles of Cases B, C, and D show an overall shape that is more consistent with the experimental results. In all but case B, we observe a clear upward spike in soot volume fraction at about $y/D = 100$; while the location does correspond to our peak temperature values, it is still unclear why this peak occurs in our simulations and not in simulations of this case performed by other groups. This is one area of continuing investigation.

In addition to the models presented here, the ODT code is continuously updated to include various other soot models; in the future, it may include PAH-based nucleation, PAH condensation mechanisms, and various advanced soot particle size distribution treatments like the method of moments with interpolative closure [32]. Current and future ODT simulations of sooting jets in the Sandia configuration and others will incorporate more advanced soot models in order to continue evaluating ODT as a tool for soot modeling.

The ODT simulation presented here represents an important step toward accurate soot representation within the framework of the one-dimensional turbulence model. While the ODT simulations currently predict soot presence one to two orders of magnitude different than other simulation approaches do, its prediction of gas temperature is similar to predictions by other groups. This is an encouraging indication that ODT, with the addition of improved soot models, may be a good complement to LES studies of soot transport and behavior. The mechanism comparison in Table 2 and Figure 3 is a simple example of the type of parametric study that ODT is uniquely capable of performing due to its relatively low computational cost, which encourages its use for future studies with greater scope.

5. Conclusion

This paper presented initial ODT simulations of a sooting, ethylene jet flame in the configuration presented by Zhang et al. [60] via the ISF Workshop Target Flames [61]. Comparison of the ODT simulations to the experimental data and other simulations of this configuration reveal that ODT may potentially be a good complement to sooting jet simulation with LES, but the simplicity of the soot chemistry models used do not permit conclusive comparisons. The present results encourage future simulations of this configuration using more advanced soot models.

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Table 2: Summary of ODT simulation configurations varying soot reaction mechanisms. LL = Leung and Lindstedt model [4]; HACA = hydrogen-abstraction acetylene addition model for surface growth and oxidation [13, 16]; NSC = surface oxidation by O_2 [19]; Neoh = surface oxidation by OH [21]; Fuchs = modified Brownian coagulation coefficient [67, 68].

	A	B	C	D
Nucleation	LL	LL	LL	LL
Surface growth	LL	HACA	HACA	LL
Oxidation	LL	HACA	NSC/Neoh	NSC/Neoh
Coagulation	LL	Fuchs	Fuchs	Fuchs

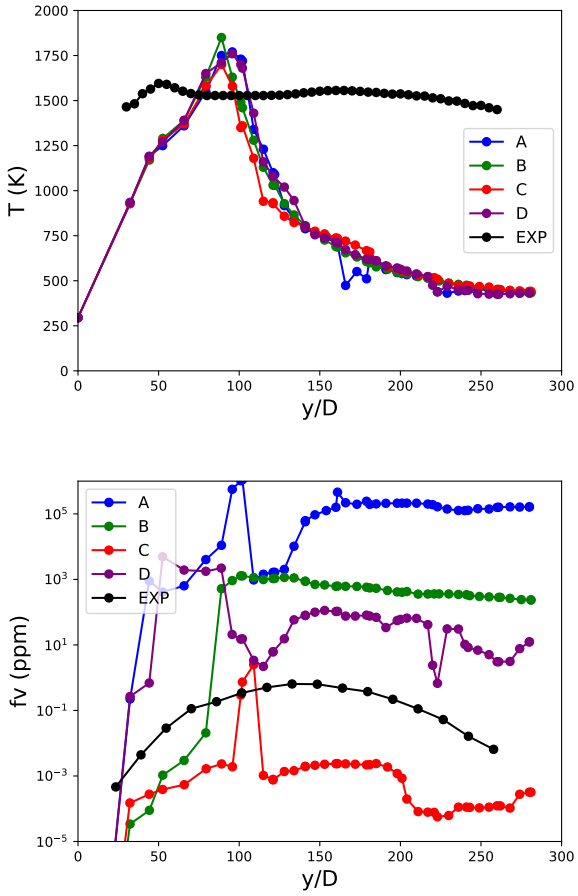

Figure 3: Results of the present ODT simulations of the Sandia ISF-4 Target Flame 2 [60] using four different combinations of soot reaction mechanisms, as detailed in Table 2

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